

Ab initio calculations of spectroscopic constants and properties of BeLi^+

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We have calculated the ground state spectroscopic constants and the molecular properties, of a molecular ion BeLi^+ , such as dipole moment, quadrupole moment and dipole polarizability at different levels of correlation: many-body perturbation theory (MP2), coupled cluster method with single and double excitations (CCSD) and CCSD with perturbative triples (CCSD(T)). The correlation consistent polarized valence cc-pVXZ (X=D, T, Q) basis sets and also their augmented counterparts are used together with the non-relativistic and relativistic Hamiltonians. The results are extrapolated to the complete basis set limit (CBS) using exponential-Gaussian function. Thus, accurate and reliable results for BeLi^+ with the most conservative error estimates on them are reported.

Keywords: Spectroscopic constants, molecular properties, potential energy curve, dipole moment, quadrupole moment, dipole polarizability, BeLi^+ .

I. INTRODUCTION

Understanding the complex structure of the molecules, neutral as well as ions, is an outstanding problem of molecular physics. With delicate investigations of such systems, one can obtain a wealth of information which can further be used to explore the various inter-related areas of research. To mention, cold and ultracold molecules can be used in the study of the controlled chemical reactions [1], the variation of fundamental physical constants such as the proton-to-electron mass ratio, $\mu \equiv m_p/m_e$ [2–4], the fine structure constant, α [4], and also in the search for the symmetry violating exotic property of an electron which hitherto has evaded detection, called the electric dipole moment (EDM) [5, 6], etc. A number of experimental techniques viz., buffer gas cooling [7] and electrostatic trapping [8] for the formation of cold molecules, photoassociation (PA) [9] and Feshbach resonance [10] for ultracold molecules, and sympathetic cooling using laser cooled atomic ions, [11–13] for molecular ions, etc., have been developed to serve this purpose. For over a decade, the neutral homonuclear and heteronuclear diatomic molecules of alkali- and alkaline-earth-metals have extensively been studied both theoretically [14–16] and experimentally [10, 17, 18]. The calculation of spectroscopic constants, permanent dipole moments (PDM's), and vibrational states of electronic ground state of monohydride ions of group IIA, IIB and Yb have been reported in [19]. Recently also, ground and first excited state of the monohydrides of alkaline-earth-metals have been investigated theoretically using multi-reference configuration interaction (MRCI) method for the purpose of laser cooling [20]. The ground and low lying excited states of MgLi and MgLi^+ have been studied using full valence configuration interaction (FCI) and MRCI methods [21]. Quite recently, the structural, electronic and dipolar properties of CaLi^+ and SrLi^+ have

also been reported in [22, 23].

Although for a simple system like BeLi^+ there is no available experimental data, to the best of our knowledge. But there exist several calculations in the literature, such as, the calculation of spectroscopic constants of $1-2^1\Sigma^+$ and $1^3\Sigma^+$ using self-consistent field (SCF) method by Sazonov *et al.* [24], stability and physicochemical reaction of this molecular species has been studied by Nicolaides *et al.* [25], the calculation of ground state spectroscopic constants at MP2 (full) level by Boldyrev *et al.* [26] using the Gaussian 92 program, calculations of the ground state and low-lying $1\Sigma^+$ electronic states of BeLi^+ by Farjallah *et al.* [27] using FCI, Rakshit *et al.* [28] reported the ground and first excited state potential energy curves (PEC's) to study the atom-ion collision at low energy and to predict the feasibility of the formation of cold molecular ion by photoassociation, ground and six low-lying excited states have been studied by Sun *et al.* [29] using MRCI + Q and multi-reference averaged quadratic coupled-cluster (MRAQCC) methods including Davidson correction. Recently, *ab initio* study of ground and low-lying excited states have been done by You *et al.* [30] using MRCI method. Very recently, Ghanmi *et al.* [31] performed the theoretical study of 44 excited electronic states of BeLi^+ molecular ion using pseudo-potential approach. In this paper, they have reported the PEC's, spectroscopic constants, dipole moment curves, and transition dipole moment curves. In the present work, for achieving reliable accuracy we have employed the higher levels of correlation methods and also we have used a successive hierarchy of three optimized basis set, so that the results can be extrapolated to the CBS limit to bring the saturation due to the size of the basis. Thus, we have calculated the spectroscopic constants, potential energy curves and dipole moment curves of BeLi^+ systematically and more accurately. In addition, we have calculated and reported the dipole polarizability and the quadrupole moment of BeLi^+ ion for the first time, known to our knowledge.

The present paper is divided into four sections. After the introduction, Section II briefly reports the method-

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ology involved in the calculations, Section III details the discussions on the calculated results and Section IV summarizes the current work.

II. METHODOLOGY

CFOUR [32] and DIRAC15 [33] software suites are used to carry out the non-relativistic and relativistic calculations, respectively, of the spectroscopic constants: equilibrium bond lengths (R_e), dissociation energies (D_e), harmonic frequencies (ω_e), anharmonic constants ($\omega_e x_e$), equilibrium rotational constants (B_e), and the molecular properties: dipole moments (μ_e), quadrupole moments (Θ_{zz}) and components of static dipole polarizability ($\alpha_{||} = \alpha_{zz}$ and $\alpha_{\perp} = \alpha_{xx}$ or α_{yy} , should z -axis be the internuclear axis of the molecule) at MP2, CCSD and CCSD(T) level of correlation. The uncontracted cc-pVXZ and aug-cc-pVXZ basis sets of Dunning *et al.* [34] with X=[D, T, Q], available in the DIRAC15 package, are used in the present calculations. The nuclear mass of 9.0121822 *au* for Be and of 7.0160030 *au* for Li have been used. Further, the point nuclear distribution and C_{2v} molecular point group symmetry are considered in our calculations. All the electrons are kept active both for diatomic constants and also for property calculations. Furthermore, the energies and PDM's are calculated for the range 2-30 Å with a step size of 1 Å and around the equilibrium point a finer step size of 0.001 Å is considered. The maximum distance of 30 Å is chosen based on the saturation of energies limited to the threshold set. The dissociation energies are evaluated by taking the difference between the energies at equilibrium bond length and those at a distance of 30 Å.

For non-relativistic calculations, the basis sets have been taken from the EMSL library [35]. The harmonic frequencies and anharmonic constants are calculated using the second-order vibrational perturbation theory, i.e., with VPT2 keyword in the CFOUR package. All calculations of the diatomic constants and of properties are carried out at zero frozen-core orbitals level and also without cutting-off any virtual orbitals. The average polarizabilities ($\bar{\alpha}$) and anisotropic polarizabilities (γ) are obtained, respectively, using:

$$\bar{\alpha} = (\alpha_{||} + 2\alpha_{\perp})/3, \quad (1)$$

and

$$\gamma = \alpha_{||} - \alpha_{\perp}. \quad (2)$$

The dipole moment of the system is calculated via first-order derivative of energy with respect to the electric field as,

$$\mu = - \left(\frac{dE}{d\epsilon} \right)_{\epsilon=0} \quad (3)$$

The z -component of the quadrupole moment, Θ_{zz} is related to the other diagonal components by the relation,

$$\Theta_{zz} = -(\Theta_{xx} + \Theta_{yy}) \quad (4)$$

and for linear molecules, $\Theta_{xx} = \Theta_{yy}$. Therefore,

$$\Theta_{zz} = -2\Theta_{xx} \quad (5)$$

For the relativistic case, the Dirac-Fock-Coulomb Hamiltonian is used with the DIRAC15 package. The contribution from the (SS|SS) integrals is taken in an approximate manner, as suggested in [36], by including an interatomic (SS|SS) correction. The energy calculations at MP2, CCSD and CCSD(T) levels are carried out with the RELCCSD module, keeping a cut-off energy of $10E_h$ for limiting the higher virtual orbitals. The diatomic constants are calculated by the second-order differentiation of the potential energy curves. The harmonic frequencies, anharmonic constants and equilibrium rotational constants, respectively, are obtained using:

$$\omega_e = \frac{1}{2\pi} \sqrt{\frac{K}{\mu}}, \quad (6)$$

$$\omega_e x_e \cong \frac{\hbar \omega_e^2}{4D_e}, \quad (7)$$

and

$$B_e = \frac{h}{8\pi^2 c \mu R_e^2}, \quad (8)$$

where K , μ and c represent the force constant, the reduced mass of the constituent atoms of a molecule and the speed of light, respectively. The calculated results are extrapolated to CBS limit using a function of the form [37, 38],

$$f(x) = f_{CBS} + B e^{-(x-1)} + C e^{-(x-1)^2} \quad (9)$$

where B and C are constant parameters, $x = 2, 3, 4$ is the cardinal number for basis sets DZ, TZ and QZ, respectively, $f(x)$ is the property calculated with the basis set characterized by cardinal number x and f_{CBS} is the complete basis set limit for the property of interest.

The estimation of the uncertainty for the calculations, in general, is a little tricky; there can be two possible error sources: one arising due to the choice or the size of the basis set and the other arising from the negligence of higher order correlation effects beyond what is considered in the present work. As we have done a series of calculations with a successive hierarchy of optimized basis sets, and extrapolated the results systematically, to the CBS limit, we least expect the error due to the choice of the basis set. As the contributions from the higher order correlation effects are not expected to be larger than that of the leading order triples considered perturbatively in our work, we have quoted the entire contribution from the latter, viz. CCSD(T) - CCSD at CBS level, as the maximum possible error bar (Δ) on our results. Thus, we recommend the final result, f_{final} , of the calculated property as,

$$f_{final} = f_{CCSD(T)} \pm (|\Delta|) \quad (10)$$

where $f_{CCSD(T)}$ is the CBS value of the property of interest at CCSD(T) level.

TABLE I. The computed spectroscopic constants for the ground state of BeLi^+ , in the non-relativistic case and the available results in the literature.

Basis	Method	R_e (au)	D_e (cm^{-1})	ω_e (cm^{-1})	$\omega_e x_e$ (cm^{-1})	B_e (cm^{-1})	α_e (cm^{-1})
DZ	SCF	5.006	5068	305	5.01	0.608	0.0138
	MP2	4.966	4994	320	4.80	0.618	0.0130
	CCSD	4.957	4644	318	4.84	0.621	0.0131
	CCSD(T)	4.955	4655	318	4.93	0.621	0.0131
TZ	SCF	5.008	5105	302	5.16	0.608	0.0139
	MP2	4.947	5145	324	4.82	0.623	0.0129
	CCSD	4.942	4799	319	4.84	0.624	0.0131
	CCSD(T)	4.940	4812	319	4.82	0.625	0.0131
QZ	SCF	5.004	5116	300	5.15	0.609	0.0144
	MP2	4.930	5222	326	4.95	0.627	0.0132
	CCSD	4.927	4859	321	4.86	0.628	0.0134
	CCSD(T)	4.923	4868	322	4.85	0.629	0.0133
CBS	SCF	5.001	5122	299	5.14	0.610	0.0147
	MP2	4.919	5269	327	5.04	0.630	0.0134
	CCSD	4.917	4894	322	4.87	0.631	0.0136
	CCSD(T)	4.912	4900	324	4.87	0.631	0.0134
Error bar		± 0.005	± 6	± 2	± 0.0006	± 0.0009	± 0.0002
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	SCF [24]	5.027	5001	320	8.2	0.601	—
	[25]	4.920	—	—	—	—	—
	MP2 [26]	4.968	—	320	—	—	—
	MP4* [26]	—	4757	—	—	—	—
	QCISD(T)** [26]	—	4617	—	—	—	—
	FCI [27]	4.96	4849	321.2	6.48	0.6395	—
	CCSD(T) [29]	4.964	—	315.5	—	0.623	—
	MRCI [30]	4.913	4903.6	318.4	4.310	0.6173	—
	FCI [31]	4.940	4862	323.7	5.45	0.6395	—
	MRD-CI*** [43]	5.083	—	—	—	—	—

* MP4 - Fourth-order many-body perturbation theory, ** QCISD(T) - Quadratic configuration interaction including singles and doubles with partial triples, *** MRD-CI - Multireference Determinant configuration interaction.

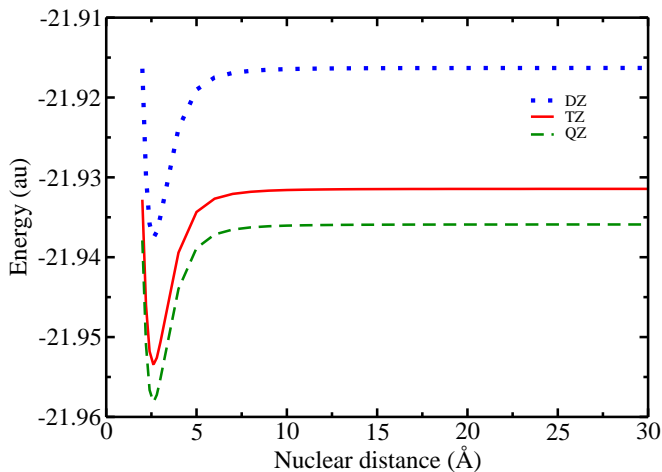


FIG. 1. (colour online) Potential energy curves for the ground state of BeLi^+ , at CCSD(T) level of correlation, in the non-relativistic case.

III. RESULTS AND DISCUSSION

Figures 1-2 show the potential energy curves for the ground state of BeLi^+ , obtained at the CCSD(T) level of correlation, using the non-relativistic and the relativistic Hamiltonian, respectively. Although we do not observe a clear trend between the two, the non-relativistic PEC's seem to be lower in energy.

The spectroscopic constants computed, using the non-relativistic Hamiltonian, at various levels of correlation considered in this work are shown in Table I. In addition, the results extrapolated to CBS limit are also shown together with the results available from the literature. Our results for the spectroscopic constants shows a good agreement with the available theoretical results [24–27, 29–31, 43]. The difference between our CBS values at SCF level and those quoted in [24] is not more than 7% in all the spectroscopic constants but anharmonic constant. The latter, which depends on other diatomic constants, shows a larger deviation. The MP2 level results of Ref. [26] also compare quite well with our results at the similar level of approximation. The results reported in [27], calculated at FCI level

TABLE II. The computed spectroscopic constants for the ground state of BeLi⁺, in the relativistic case..

Basis	Method	R_e (au)	D_e (cm ⁻¹)	ω_e (cm ⁻¹)	$\omega_e x_e$ (cm ⁻¹)	B_e (cm ⁻¹)
DZ	SCF	5.006	5067	303	4.53	0.609
	MP2	4.964	5009	327	5.35	0.619
	CCSD	4.955	4660	310	5.17	0.621
	CCSD(T)	4.953	4671	323	5.60	0.622
TZ	SCF	5.006	5104	306	4.59	0.609
	MP2	4.947	5196	323	5.03	0.624
	CCSD	4.944	4847	319	5.26	0.624
	CCSD(T)	4.940	4860	311	5.00	0.625
QZ	SCF	5.004	5115	356	6.06	0.610
	MP2	4.919	5305	334	5.25	0.631
	CCSD	4.913	4955	318	5.10	0.632
	CCSD(T)	4.910	4965	331	5.53	0.633
CBS	SCF	5.002	5121	390	7.05	0.611
	MP2	4.901	5372	342	5.41	0.635
	CCSD	4.892	5022	317	4.99	0.637
	CCSD(T)	4.890	5019	345	5.91	0.638
Error bar		±0.002	±3	±28	±0.92	±0.001

and our recommended CCSD(T) results, highlighted in bold fonts, agree extremely well. According to the spectroscopy study of Sun *et al.* [29] at CCSD(T) level, BeLi⁺ molecular ion has equilibrium distance $R_e = 4.964$ au, harmonic frequency $\omega_e = 315.5$ cm⁻¹, and rotational constant $B_e = 0.623$ cm⁻¹, which are close to our result of 4.912 au, 324 cm⁻¹ and 0.631 cm⁻¹ respectively, at same level of correlation. Except the anharmonic constant, which is 0.56 cm⁻¹ larger than that of You *et al.* [30], and 0.58 cm⁻¹ smaller than that of Ghanmi *et al.* [31], the difference between our CBS results at CCSD(T) level and those reported in Ref. [30, 31] at MRCI and FCI level of correlation respectively, is less than 3% in all diatomic constants. The results of the similar calculations, performed for the sake of completion, using the relativistic Hamiltonian are given in Table II. As is obvious, due to the small charge of Be and Li, we did not observe an appreciable difference between the relativistic and the non-relativistic results in all the spectroscopic constants.

The computed results, using the non-relativistic Hamiltonian, of molecular properties such as dipole moments, quadrupole moments, components of static dipole polarizability, isotropic and anisotropic polarizabilities, and parallel-component of the dipole polarizabilities at super molecular limit (100 au) symbolized as α_{100} , are tabulated in Table III. Knowledge of dipole moment is useful for the study of electric dipole-dipole interactions, quantum computing, etc. [39, 40]. Figure 3 shows the PDM as a function of internuclear distance R at CCSD(T) level of correlation using cc-pVQZ basis set. The dipole moment curve shows almost linear behaviour from 6 Å to 30 Å. In this figure, we have compared our results with the results reported by Farjallah *et al.* [27]. The excess of negative charge on the lighter

atom is confirmed by the negative values of dipole moment, with the assumption that the orientation of the interatomic axis is from lighter to heavier element. We have, however, plotted the absolute values of dipole moment against R . The dipole polarizability describes the behaviour of a molecule in the presence of electric field and hence, the dipole polarizability is an important property for the study of the optical properties of materials, intermolecular forces, etc. As we move towards the higher basis set, most of the results for spectroscopic constants and molecular properties converge.

The augmentation of the basis sets with diffuse functions does not appreciably alter the results of the spectroscopic constants and the molecular properties. The differences in our final results between the augmented and un-augmented basis sets is about, 0.001 au in R_e , 1 cm⁻¹ in D_e and ω_e , 0.2 cm⁻¹ in $\omega_e x_e$, 0.0003 cm⁻¹ in B_e , 0.0001 cm⁻¹ in α_e , 0.0004 au in μ_e and Θ_{zz} , 0.066 au in $\bar{\alpha}$, and 0.051 au in γ , at the CCSD(T) level. However, the polarizability results, with and without augmentation, in the super-molecular limit seem to have a noticeable difference. At the CCSD(T) level, the CBS value of $\alpha_{100} = (37.944 \pm 0.167)$ au with augmented basis set, while $\alpha_{100} = (37.085 \pm 0.189)$ au without augmentation. The former is significantly close to the the sum of polarizabilities of the Be [41] and Li⁺ [42], $\alpha_A \simeq \alpha_{Be} + \alpha_{Li^+} = 37.71 + 0.191 = 37.901$ au. Due to the the unavailability of experimental value of polarizability for Li⁺ in the literature, we have taken its calculated value at the CCSD(T) level from [42] and combined with the experimental value for Be.

TABLE III. Dipole moment, quadrupole moment, components of dipole polarizability at equilibrium point, and polarizability at super-molecular limit, for the ground state of BeLi^+ .

Basis	Method	$ \mu_e $ (au)	Θ_{zz} (au)	α_{\parallel} (au)	α_{\perp} (au)	$\bar{\alpha}$ (au)	γ (au)	α_{100} (au)
DZ	SCF	1.274	12.642	46.086	36.843	43.005	9.243	44.586
	MP2	1.335	12.713	43.881	34.285	37.483	9.596	40.403
	CCSD	1.449	11.732	42.010	32.071	35.384	9.939	35.921
	CCSD(T)	1.450	11.712	41.942	32.006	35.318	9.936	35.838
TZ	SCF	1.276	12.622	45.941	36.713	42.865	9.228	45.520
	MP2	1.310	12.130	43.652	34.306	37.421	9.346	41.348
	CCSD	1.421	11.711	42.223	32.347	35.639	9.876	37.012
	CCSD(T)	1.422	11.687	42.143	32.273	35.563	9.870	36.911
QZ	SCF	1.274	12.621	45.895	36.745	42.845	9.150	45.721
	MP2	1.291	12.097	43.499	34.407	37.438	9.092	41.572
	CCSD	1.405	11.680	42.197	32.466	35.710	9.731	37.191
	CCSD(T)	1.406	11.645	42.087	32.363	35.604	9.724	37.037
CBS	SCF	1.273	12.621	—	—	42.836	9.098	45.826
	MP2	1.279	12.095	—	—	37.452	8.929	41.691
	CCSD	1.395	11.660	—	—	35.749	9.635	37.274
	CCSD(T)	1.396	11.617	—	—	35.623	9.628	37.085
Error bar		± 0.001	± 0.043	—	—	± 0.126	± 0.007	± 0.189

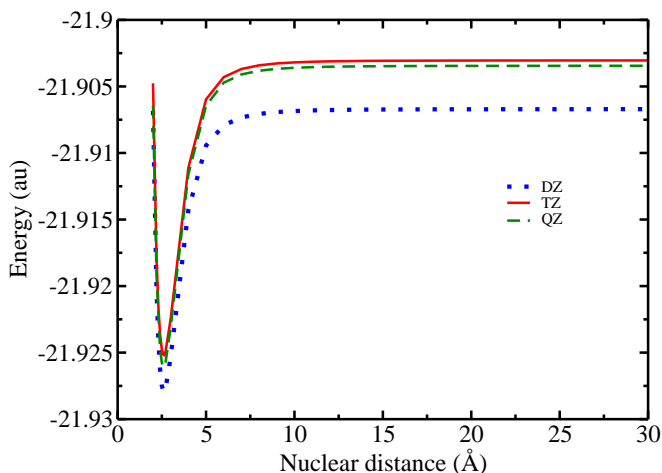


FIG. 2. (colour online) Potential energy curves for the ground state of BeLi^+ , at the CCSD(T) level of correlation, in the relativistic case.

IV. SUMMARY

In summary, we have carried out the *ab initio* calculations of the spectroscopic constants and the molecular properties of the ground state ($^1\Sigma^+$) of BeLi^+ molecular ion dissociating into $\text{Be} + \text{Li}^+$. The objective of this paper is to systematically improve the accuracies of the hitherto existing results. The saturation of the results with respect to the size of the basis sets and the higher levels of correlations are investigated. Our findings of diatomic constants and dipole moment are in reasonably good agreement with the available results in the literature. Other properties such as the dipole polarizability

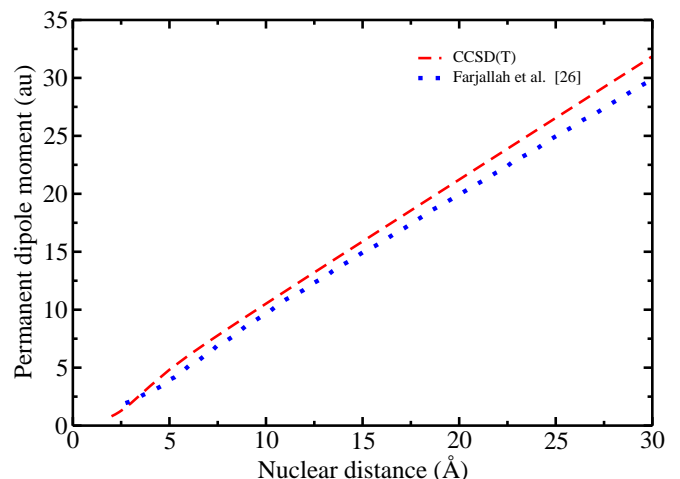


FIG. 3. (colour online) Permanent dipole moment curve using QZ basis set at CCSD(T) level of correlation.

and the quadrupole moment for this ion are reported for the first time, in this work, to the best of our knowledge. We have reported very conservative error estimates on our results by considering the entire perturbative triples contribution as the maximum possible error.

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